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**Ruthenium(II) and osmium(II) polypyridyl complexes of an asymmetric pyrazinyl- and pyridinyl-containing 1,2,4-triazole based ligand. Connectivity and physical properties of mononuclear complexes**

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*Published in:*  
Journal of the Chemical Society, Dalton Transactions

*DOI:*  
[10.1039/b206667j](https://doi.org/10.1039/b206667j)

**IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.**

*Document Version*  
Publisher's PDF, also known as Version of record

*Publication date:*  
2002

[Link to publication in University of Groningen/UMCG research database](#)

*Citation for published version (APA):*

Browne, W. R., O'Connor, C. M., Hughes, H. P., Hage, R., Walter, O., Doering, M., Gallagher, J. F., & Vos, J. G. (2002). Ruthenium(II) and osmium(II) polypyridyl complexes of an asymmetric pyrazinyl- and pyridinyl-containing 1,2,4-triazole based ligand. Connectivity and physical properties of mononuclear complexes. *Journal of the Chemical Society, Dalton Transactions*, (21), 4048-4054.  
<https://doi.org/10.1039/b206667j>

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'Wesley R. Browne'
'Manfred Doering'
'J. F. Gallagher'
'Ronald Hage'
'Helen P. Hughes'
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#=====
# 3. TITLE AND AUTHOR LIST

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Ruthenium(II) and Osmium(II) Polypyridyl Complexes of asymmetric
pyrazinyl- and pridinyl-1,2,4-triazole based ligands.
Part 1: Connectivity and physical properties of mononuclear complexes.
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C27 0.0247(9) 0.0242(10) 0.0271(10) -0.0016(8) 0.0013(8) 0.0097(8)
C28 0.0306(11) 0.0313(11) 0.0363(12) -0.0055(9) 0.0011(9) 0.0159(9)
C29 0.0353(12) 0.0241(10) 0.0496(14) -0.0024(10) -0.0024(10) 0.0157(9)
C30 0.0370(12) 0.0226(10) 0.0423(13) 0.0047(9) 0.0009(10) 0.0091(9)
C31 0.0285(10) 0.0246(10) 0.0333(11) 0.0034(8) 0.0054(9) 0.0089(8)
O100 0.101(2) 0.162(3) 0.096(2) 0.040(2) 0.0257(19) 0.080(2)
C100 0.137(4) 0.106(3) 0.080(3) 0.043(3) 0.042(3) 0.083(3)

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\_geom\_special\_details

;

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

;

loop\_

\_geom\_bond\_atom\_site\_label\_1

\_geom\_bond\_atom\_site\_label\_2

\_geom\_bond\_distance

\_geom\_bond\_site\_symmetry\_2

\_geom\_bond\_publ\_flag

Ru1 N2 2.0398(16) . ?

Ru1 N8 2.0488(17) . ?

Ru1 N9 2.0525(17) . ?

Ru1 N10 2.0579(16) . ?

Ru1 N7 2.0603(16) . ?

Ru1 N1 2.1033(17) . ?

P1 F14 1.5823(16) . ?

P1 F13 1.5925(15) . ?

P1 F15 1.5963(15) . ?

P1 F16 1.5991(15) . ?

P1 F12 1.6053(15) . ?

P1 F11 1.6132(15) . ?

N1 C1 1.343(3) . ?

N1 C5 1.363(3) . ?

N2 C6 1.348(3) . ?

N2 N3 1.355(2) . ?

N3 C7 1.348(3) . ?

N4 C6 1.340(3) . ?

N4 C7 1.356(3) . ?

N5 C11 1.338(3) . ?

N5 C8 1.340(3) . ?

N6 C9 1.333(3) . ?

N6 C10 1.336(3) . ?

N7 C12 1.342(3) . ?

N7 C16 1.362(3) . ?

N8 C21 1.349(3) . ?

N8 C17 1.359(2) . ?

N9 C22 1.351(3) . ?

N9 C26 1.366(3) . ?

N10 C31 1.345(3) . ?

N10 C27 1.365(3) . ?

C1 C2 1.380(3) . ?

C2 C3 1.381(3) . ?

C3 C4 1.387(3) . ?  
C4 C5 1.385(3) . ?  
C5 C6 1.458(3) . ?  
C7 C8 1.470(3) . ?  
C8 C9 1.393(3) . ?  
C10 C11 1.381(3) . ?  
C12 C13 1.382(3) . ?  
C13 C14 1.379(3) . ?  
C14 C15 1.383(3) . ?  
C15 C16 1.387(3) . ?  
C16 C17 1.474(3) . ?  
C17 C18 1.391(3) . ?  
C18 C19 1.379(3) . ?  
C19 C20 1.384(3) . ?  
C20 C21 1.378(3) . ?  
C22 C23 1.380(3) . ?  
C23 C24 1.380(4) . ?  
C24 C25 1.382(4) . ?  
C25 C26 1.386(3) . ?  
C26 C27 1.474(3) . ?  
C27 C28 1.387(3) . ?  
C28 C29 1.383(3) . ?  
C29 C30 1.379(3) . ?  
C30 C31 1.387(3) . ?  
O100 C100 1.396(5) . ?

loop\_  
\_geom\_angle\_atom\_site\_label\_1  
\_geom\_angle\_atom\_site\_label\_2  
\_geom\_angle\_atom\_site\_label\_3  
\_geom\_angle  
\_geom\_angle\_site\_symmetry\_1  
\_geom\_angle\_site\_symmetry\_3  
\_geom\_angle\_publ\_flag  
N2 Ru1 N8 96.92(6) . . ?  
N2 Ru1 N9 173.35(7) . . ?  
N8 Ru1 N9 88.76(7) . . ?  
N2 Ru1 N10 96.79(6) . . ?  
N8 Ru1 N10 98.70(7) . . ?  
N9 Ru1 N10 78.87(7) . . ?  
N2 Ru1 N7 87.28(6) . . ?  
N8 Ru1 N7 78.72(7) . . ?  
N9 Ru1 N7 97.25(7) . . ?  
N10 Ru1 N7 175.45(6) . . ?  
N2 Ru1 N1 77.98(6) . . ?  
N8 Ru1 N1 173.94(6) . . ?  
N9 Ru1 N1 96.54(7) . . ?  
N10 Ru1 N1 85.25(6) . . ?  
N7 Ru1 N1 97.64(6) . . ?  
F14 P1 F13 91.09(10) . . ?  
F14 P1 F15 91.50(10) . . ?  
F13 P1 F15 90.41(9) . . ?  
F14 P1 F16 90.72(10) . . ?  
F13 P1 F16 178.13(10) . . ?  
F15 P1 F16 90.05(9) . . ?  
F14 P1 F12 89.82(9) . . ?  
F13 P1 F12 89.70(8) . . ?  
F15 P1 F12 178.68(9) . . ?  
F16 P1 F12 89.80(9) . . ?  
F14 P1 F11 178.98(10) . . ?  
F13 P1 F11 89.24(9) . . ?  
F15 P1 F11 89.47(9) . . ?  
F16 P1 F11 88.94(9) . . ?  
F12 P1 F11 89.22(8) . . ?  
C1 N1 C5 117.75(18) . . ?  
C1 N1 Ru1 126.61(15) . . ?



C5 N1 Ru1 115.45(13) . . ?  
C6 N2 N3 107.46(16) . . ?  
C6 N2 Ru1 116.13(13) . . ?  
N3 N2 Ru1 135.86(13) . . ?  
C7 N3 N2 103.64(16) . . ?  
C6 N4 C7 100.82(16) . . ?  
C11 N5 C8 115.9(2) . . ?  
C9 N6 C10 115.8(2) . . ?  
C12 N7 C16 118.22(17) . . ?  
C12 N7 Ru1 125.85(14) . . ?  
C16 N7 Ru1 115.91(13) . . ?  
C21 N8 C17 118.03(18) . . ?  
C21 N8 Ru1 125.76(14) . . ?  
C17 N8 Ru1 116.19(13) . . ?  
C22 N9 C26 118.09(18) . . ?  
C22 N9 Ru1 125.82(15) . . ?  
C26 N9 Ru1 115.95(14) . . ?  
C31 N10 C27 118.25(17) . . ?  
C31 N10 Ru1 125.94(14) . . ?  
C27 N10 Ru1 115.49(13) . . ?  
N1 C1 C2 122.8(2) . . ?  
C1 C2 C3 119.4(2) . . ?  
C2 C3 C4 118.8(2) . . ?  
C5 C4 C3 119.1(2) . . ?  
N1 C5 C4 122.20(19) . . ?  
N1 C5 C6 113.20(17) . . ?  
C4 C5 C6 124.58(19) . . ?  
N4 C6 N2 113.06(17) . . ?  
N4 C6 C5 130.20(18) . . ?  
N2 C6 C5 116.74(17) . . ?  
N3 C7 N4 115.01(17) . . ?  
N3 C7 C8 122.04(18) . . ?  
N4 C7 C8 122.92(18) . . ?  
N5 C8 C9 120.96(19) . . ?  
N5 C8 C7 118.29(18) . . ?  
C9 C8 C7 120.74(19) . . ?  
N6 C9 C8 122.9(2) . . ?  
N6 C10 C11 121.7(2) . . ?  
N5 C11 C10 122.8(2) . . ?  
N7 C12 C13 122.5(2) . . ?  
C14 C13 C12 119.2(2) . . ?  
C13 C14 C15 119.2(2) . . ?  
C14 C15 C16 119.0(2) . . ?  
N7 C16 C15 121.83(19) . . ?  
N7 C16 C17 114.32(17) . . ?  
C15 C16 C17 123.85(18) . . ?  
N8 C17 C18 121.80(19) . . ?  
N8 C17 C16 114.80(17) . . ?  
C18 C17 C16 123.39(18) . . ?  
C19 C18 C17 119.4(2) . . ?  
C18 C19 C20 118.9(2) . . ?  
C21 C20 C19 119.4(2) . . ?  
N8 C21 C20 122.5(2) . . ?  
N9 C22 C23 122.7(2) . . ?  
C24 C23 C22 119.0(2) . . ?  
C23 C24 C25 119.2(2) . . ?  
C24 C25 C26 119.6(2) . . ?  
N9 C26 C25 121.4(2) . . ?  
N9 C26 C27 114.42(17) . . ?  
C25 C26 C27 124.1(2) . . ?  
N10 C27 C28 121.5(2) . . ?  
N10 C27 C26 114.44(17) . . ?  
C28 C27 C26 124.10(19) . . ?  
C29 C28 C27 119.5(2) . . ?  
C30 C29 C28 119.0(2) . . ?  
C29 C30 C31 119.2(2) . . ?

N10 C31 C30 122.4(2) . . ?

|                                           |        |
|-------------------------------------------|--------|
| _diffraction_measured_fraction_theta_max  | 0.945  |
| _diffraction_reflns_theta_full            | 28.30  |
| _diffraction_measured_fraction_theta_full | 0.945  |
| _refine_diff_density_max                  | 0.702  |
| _refine_diff_density_min                  | -0.524 |
| _refine_diff_density_rms                  | 0.064  |